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Book of Abstracts
November 2-5, 1998

Kellie Ann Beall, Editor

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Gaithersburg, Maryland 20899

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U.S. Department of Commerce
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Technology Administration
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Center for the Simulation of Accidental Fires & Explosions at University of Utah: An Overview

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The University of Utah in an alliance with the DOE Accelerated Strategic Computing Initiative (ASCI) created the Center for the Simulation of Accidental Fires and Explosions (C-SAFE) to focus specifically on providing state-of-the-art, science-based tools for the numerical simulation of accidental fires and explosions, especially within the context of handling and storage of highly flammable materials. The objective of the C-SAFE is to provide a system comprising a problem-solving environment in which fundamental chemistry and engineering physics are fully coupled with non-linear solvers, optimization, computational steering, visualization and experimental data verification. The availability of simulations using this system will help to better evaluate the risks and safety issues associated with fires and explosions. Our team will integrate and deliver a system that will be validated and documented for practical application to accidents involving both hydrocarbon and energetic materials.

Although the ultimate C-SAFE goal is to simulate fires involving a diverse range of accident scenarios including multiple high-energy devices, complex building/surroundings geometries and many fuel sources, the initial efforts will focus on the computation of a scenario of slow and .rapid heating of a container with conventional explosives in a pool fire (e.g., a container of high explosives involved in an intense jet-fuel fire after an airplane crash).

These large-scale problems require consideration of fundamental gas and condensed phase chemistry, structural mechanics, turbulent reacting flows, convective and radiative heat transfer, and mass transfer, in a time-accurate, full-physics simulation of accidental fires. This simulation will be expansive enough to include the physical and chemical changes in containment vessels and structures, the mechanical stress and rupture of the container, and the chemistry and physics of organic, metallic and energetic material inside the vessel. We will include deflagration-to-detonation transitions (DDT) of any energetic material in the fire, but the simulation will end when/if detonation occurs. C-SAFE will provide coupling of the micro-scale and meso-scale contributions to the macroscopic application in order to provide full-physics across the breadth of supporting mechanistic disciplines, and to achieve efficient utilization of ASCI program supercomputers.

We will utilize a simulation development roadmap (SDRM) consisting of distinct, sequential steps, which parallel the events in our physical problem: Fire Spread Following a Prescribed Ignition, Container Dynamics and High Energy Transformations. A fire or explosion is initiated by an ignition; depending on the magnitude of heat generation and dissipative terms, a perturbation by an ignition source either decays or grows into a flame, followed by a spreading fire and possibly explosion. The fire or explosion can cause the container of HE material to undergo changes, perhaps rupture and, simultaneously or sequentially, the HE material itself can undergo transformations which lead to an explosion. The overall mission is to integrate these computational steps into a coupled fire and explosion system. To fulfill this mission we will draw on three core disciplines available at the University: molecular fundamentals, computational engineering, and computer science.

The thrust of the molecular fundamentals team will be to perform micro-scale analyses of physical and chemical processes. To this end, they will be concerned with aspects of molecular dynamics, electronic structure, and statistical mechanics in an integrated fashion to dynamically obtain properties for all materials (condensed phases, vaporized phases, and structures) in the fire and explosion. The thrust of the computational engineering team will be to develop meso-scale models that bridge the ranges of length and time scales between microscopic and macroscopic properties. They will also develop large-scale Eulerian and Lagrangian models to describe structural and transport processes with geometric and mechanistic fidelity. The computer science effort will focus on a system development framework which combines target architecture performance analysis tools at the lowest level with an integrated, higher level scientific problem solving environment to provide interactive computational steering, visualization and large data set analysis capabilities.

University of Utah faculty have joined with strategically selected faculty from nearby Brigham Young University and Utah State University and experimental scientists from Cordant Technologies (formerly Thiokol Corporation) to create C- SAFE. A tightly integrated structure has been set up to simultaneously ensure that (1) the common objective of developing a verified, fire and explosive simulation system is attained and (2) modern scientific/computational techniques are used throughout. Decisions regarding selection of key components to integrate into each step will be based on nonlinear sensitivity analysis and numerical optimization of our overall accidental fire simulation. The C-SAFE system requires a computational infrastructure that can support multi-physics modeling of large- scale, complex phenomena. C-SAFE models the physical complexities from the molecular level of HE materials, through millimeter-sized representations of the container, to the meter-sized representations of the fire spread. At each of these levels, the simulations will involve up to 109 discrete mesh points. Due to the multiple scales, the spatial requirements may exceed the terabyte range for the full simulation. The computation will also require 1010 time-steps to compute the physical time scales ranging from microseconds to minutes or hours. Thus the storage requirements far exceed the capacities of most computing facilities. Not only are the memory and storage requirements at the terascale, the computational demands are also on the order of tens to hundreds of teraflops. When these requisites are compounded with the visualization needs, successful realization of the C-SAFE system involves dataset management, model building, simulation, and visualization at the Terascale level.

The C-SAFE system will be validated by comparison with experimental data for a variety of conditions at four different levels: fundamental rates and submodels; individual and coupled SDRM steps; well-defined, integrated multistep experiments; actual, full-scale fires and explosions. Initially, the primary focus will be on utilizing existing data, especially from the National Labs, fire research laboratories, and Cordant. Additional, detailed data to validate the C-SAFE computations will be carried out at the University supplemental tests with high energy materials at Cordant.